Hybrid Monte Carlo Without Pseudofermions

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We introduce a dynamical fermion algorithm which is based on the hybrid Monte Carlo (HMC) algorithm, but without pseudofermions. The molecular dynamics steps in HMC are retained except the derivatives with respect to the gauge fields are calculated with the Z_2 noise. The determinant ratios are estimated with the Padè - Z_2 method. Finally, we use the Kennedy-Kuti linear accept/reject method for the Monte Carlo step which is shown to respect detailed balance. We comment on the comparison of this algorithm with the pseudofermion algorithm.

1. Introduction

The partition function of the gauge field theory with dynamical fermions in the Euclidean path-integral formalism has the following generic form

$$Z = \int [dU] det M[U] e^{-S_G} \tag{1}$$

where S_G is the pure gauge part of the action and U is the link variable. The Grassmann numbers representing the fermions are formally intergrated out to give a fermion determinant. Since the determinant is very non-local, the Monte Carlo algorithms with dynamical fermions is known to be very time-consuming. The best algorithm so far is the Hybrid Monte Carlo [1] which introduces a Monte Carlo step to the hybrid (molecular/hybrid) algorithm to remove the discretization error from the molecular dynamics step. This algorithm avoids calculating the determinant directly by introducing pseudofermion variables. The partition then takes the form

$$Z = \int [dU][d\chi^*][d\chi] e^{-S_G - \chi^*(M^\dagger M)^{-1}\chi} \tag{2}$$

where χ is the pseudofermion field variable.

In this paper, we shall present an algorithm which estimates the determinant ratio directly without using pseudofermions. To begin with, we note that the determinant can be written as $e^{Tr \log M}$ and the trace can be estimated by the Z_2 noise [2] which is known to yield the minimum

variance [3]. Thus the partition in eq. (1) takes the form

$$Z = \int [dU] e^{-S_G + \int dz_2 \, z_2 (\log M) z_2} \tag{3}$$

where z_2 is the Z_2 noise for estimating the trace of the matrix $\log M$.

2. Estimating Determinants with Padè-Z_2 Method

It has been shown that there is an efficient algorithm to estimate the determinant by expanding the $\log M$ using the Padè approximation. The trace is then estimated by the Z_2 noise. This is reported by Chris Thron [4]. The expectation value of the $\log det M$ can be written as

$$E[\log det M] = E[Tr \log M] \sim \frac{1}{N} \sum_{i,j} z_2^j (\frac{b_i}{M + c_i I}) z_2^j \tag{4}$$

where b_i and c_i are constants. It is worthwhile noting that since we will use this estimate for the determinant ratios in the Monte Carlo step for the two matrices M_1 and M_2 whose eigenvalues are close to each other, we can do the Padè expansion aroud 1 with a small set of b_i and c_i. As long as there is enough memory, the matrix inversion with the set of b_i and c_i can be done with the minimum residual with about 8% overhead in CPU time as compared with inversion of the one with the smallest diagonal term (the equivalent of the quark mass) [5–7]. Furthermore, c_i are real and positive so that the matrix $M + c_i I$ is better

conditioned then M itself. Finally, we should caution that the PZ method does not work if there are real negative eigenvalues, because the log has a cut on the negative real axis.

3. Hybrid Monte Carlo with PZ Determinant

The algorithm we propose involves two steps:
1. **Molecular Dynamics with Determinant Force:**

The molecular dynamics step is retained as in HMC, except the pseudofermion force is replaced with the determinant force in the evolution equations.

$$\pi(\frac{\delta\tau}{2}) = \pi(0) - T[\frac{\partial S_G}{\partial U}(0)U(0)]\frac{\delta\tau}{2}$$
$$+ z_2 T[\frac{\partial \log M}{\partial U}(0)U(0)]z_2\frac{\delta\tau}{2}$$
$$U(\delta\tau) = exp[\pi(\frac{\delta\tau}{2})\delta\tau]U(0)$$
$$\pi(\delta\tau) = \pi(\frac{\delta\tau}{2}) - T[\frac{\partial S_G}{\partial U}(\delta\tau)U(\delta\tau)]\frac{\delta\tau}{2}$$
$$+ z_2 T[\frac{\partial \log M}{\partial U}(\delta\tau)U(\delta\tau)]z_2\frac{\delta\tau}{2} \qquad (5)$$

Several comments are ready:

The leapfrog scheme is adopted for this step as in HMC to make it reversible and area preserving. There is a discretization error $N_{MD}O(\delta\tau^3) = O(\delta\tau^2)$ as in HMC. Like the pseudofermion variable in HMC, z_2 is kept fixed during the MD trajectory.

2. **Monte Carlo:**

In lieu of the Metropolis accept/reject criteria, we shall us the Kennedy-Kuti linear test [8]

$$P(V \longleftarrow U) = \begin{cases} \frac{1}{2} & \text{if } U > V \\ \langle\frac{R}{2}\rangle_{z_2} & \text{if } U \leq V \end{cases}$$

where U and V are two configurations and $R = e^{-\delta H}$. H is molecular dynamics hamiltonian. We note that this satisfies detailed balance provided R is an unbiased estimate [8]. Since the estimate of δH is unbiased with the Z_2 noise, we can use the Bhanot-Kennedy algorithm [9] to turn R into an unbiased estimate:

Suppose x is an unbiased estimate,

$$e^x = 1 + x + \frac{1}{2}(x^2 + \frac{1}{3}(x^3 + ...$$
$$\langle e^{\hat{x}} \rangle = e^x \qquad (6)$$

4. Comparison with HMC with Pseudofermions

We shall point out several apparent differences between the pseudofermion algorithm and the current determinant algorithm and will make some preliminary comparison of the two approaches.
1. **MD trajectories:**

The pseudofermion approach requires two matrix inversions $\longrightarrow M^\dagger M x = \chi$ in each step. Whereas, the determinant approach reqires only one such inversion in $\longrightarrow Mx = z_2$. Accuracy of the residual of matrix inversion is needed for reversibility for both approaches, i.e.

$$\langle e^{-\delta H} \rangle = 1 \qquad (7)$$

where the average is over all the trajectories. This allows one to test the thermal equilibrium and make a comparison of the two approaches.
2. **Overhead of Determinant Algorithm in Accept/Reject Step:**

The Bhanot-Kennedy unbiased estimate in eq. (6), needs on the average e terms in the matrix inversion to have independent estimate of δH. It may be desirable to have more than one Z_2 noise in the estimate of the determinant ratio.

In the Kennedy-Kuti linear accept/reject test, the ratio R should lie between 0 and 2 to be a probability. This, however, can be violated in practice [9]. To make sure that the systematic errors due to the violation of $0 < R < 2$ is small, say less than 0.1%, one needs to have small enough step size in the MD trajectories.
3. **Intrinsic Noisiness:**

The ultimate test between different algorithms will be conducted by comparing how fast observables decorrelate. This will be done next. In the meantime, we shall concentrate on the issue of intrinsic noisiness. While the pseudofermion method gives the joint probability of gauge fields and pseudofermion fields, the determinant method has built in it the fluctuation of

the Z_2 noise. We shall explore the intrinsic noisiness by computing $detM_1/detM_2$ for a fixed pair of M_1 and M_2 separated by heatbath update of 20 links on a $16^3 \times 24$ lattice with $\kappa = 0.154$ with the two different methods.

In the pseudofermion method, the determinant ratio is estimated by

$$detM_1/detM_2 \sim \frac{1}{N} \sum_{i=1}^{N} e^{-\chi_i^*(M_2^\dagger M_2)^{-1}\chi_i - \eta_i^2} \qquad (8)$$

where $\chi_i = M_1^\dagger \eta_i$. In the PZ method , the determinant ratio is estimated by

$$log(\frac{detM_1}{detM_2}) \sim \frac{1}{N} \sum_{i=1}^{N} \sum_{j=1}^{L} z_2^j (\frac{b_i}{M_1/M_2 + c_i}) z_2^j \quad (9)$$

We plot in Fig. 1 and Fig. 2 the distribution of $log(detM_1/detM_2) - \langle log(detM_1/detM_2)\rangle$ for 50 gaussian and Z_2 noises respectively. We see that the distribution of the pseudofermion method is wider than that of the PZ method. We also plot in Fig. 3 the Jackknife errors of $log(detM_1/detM_2)$ due to the two method as a function of the number of noise. Again we see that the PZ method yields smaller error than that of the pseudofermion method.

Extensive tests are needed to check the efficiency of this algorithm before we can tell if this algorithm will turn out to a useful one.

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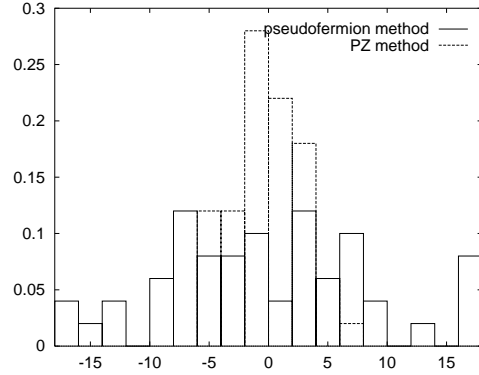7. H. P. Ying, S. J. Dong, and K. F. Liu, this proceeding.

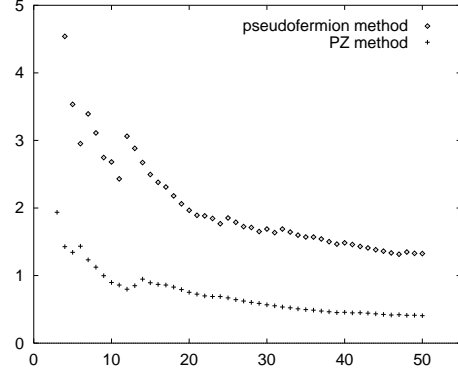Figure 1. distributions of $log(detM_1/detM_2) - \langle log(detM_1/detM_2)\rangle$ dor gaussian and Z_2 noises

Figure 2. Jackknife errors of $log(detM_1/detM_2)$

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